REMARKS

Applicants thank Examiner Sheinberg and Primary Examiner Marschel for their time and courtesy extended to Applicants' Representative during the personal interview on October 3, 2001, wherein the Examiner's Action mailed June 5, 2001, was discussed. As agreed, the following comments are submitted in response to the outstanding matters.

Extension of Time

A Petition has been filed under the provisions of 37 CFR §1.136 for an extension of time to respond to the Examiner's Action of June 5, 2001. The appropriate fee set forth in 37 CFR § 1.17 is filed herewith.

Claim Rejections - 35 USC § 112 first and second paragraphs

In order to advance the prosecution, claims 1 and 18-20 have been amended to more particularly point out the invention and to conform with U.S. Patent practice. Claims 1-20 are pending in the application.

With respect to the objection and subsequent rejection under the first paragraph, Applicants offer the following comments:

(1) For the understanding of the probe points, parts of the specification are presented with portions showing specific features of the invention underlined.

"First, in the FRAU, a molecule surrounding surface 20 (see FIG. 1 (e)) is set so as to be reflected in the spatial dimension of a molecule. This molecule surrounding surface 20 may also be set as, e.g., a surrounding surface for surrounding a molecule surrounding space formed by a so-called frontier molecular orbital of the molecule. Alternatively, the molecule surrounding surface 20 may be set as an outermost contour enveloping surface formed by a plurality of atomic spherical surfaces 4, as will be described in detail later.

The molecule surrounding space 21 (see FIG. 1 (e)) surrounded by the molecule surrounding surface 20 is divided into a plurality of component spaces 22 (see FIG. 1 (e)) in accordance with a predetermined space dividing procedure. Each of the component spaces 22 is a space unit, by which the reaction characteristic of the molecule is characterized. It is assumed that the contour surfaces surrounding the component spaces 22 are component surrounding surfaces 23, and a portion of each of the component surrounding surfaces 23 on the molecule surrounding surface 20 is a frontier surrounding surface 5 (see FIG. 1 (e)) of each of the component spaces 22.

When the molecule surrounding surface 20 is an outermost contour surrounding surface formed by the atomic spherical surfaces 4 of a plurality of atoms of a molecule, when a frontier spherical surface is adopted as the frontier surrounding surface

[20] 5 and when the number of probe points existing on the frontier spherical surface is adopted as a space occupied rate, the Preferred embodiment of the present invention will be described below. ···

"As shown in FIG. 1(a), a molecule 1, the reaction of which is to be predicted, schematically consists of a plurality of atoms 2a, 2b, 2c, ···, which are bonded to each other by lattices.

In FIG. 1 (b), reference number 3 denotes a spherical surface of van der Waals radius, which extends around the atomic center of an atom 2a and which has a van der Waals radius of, e.g., 1 through 2 angstroms. Similarly, spherical surfaces of van der Waals radius for other atoms of the molecule 1 are also shown.

In the FRAU of the present invention, the atomic spherical surface 4, which extends around the atomic center of the atom 2a and which has a radius greater than or equal to the van der Waals radius, is first described as shown in FIG. 1(b). The radius of the atomic spherical surface 4 is the van der Waals radius itself of each of the atoms, or a radius obtained by commonly adding a predetermined thickness, e.g., 0.1 angstroms, to the van der Waals radius of each of the atoms.

The atomic spherical surface 4 is described for all of the atoms 2a, 2b, 2c, ··· of the molecule 1.

As shown in FIGS. 1(c) and 1 (d), it is assumed that a portion of the atomic spherical surface 4 of each of the atoms intersecting the atomic spherical surfaces of other atoms is an interior spherical surface 6 and that a portion of the atomic spherical surface 4 other than the interior spherical surface 6 is a frontier spherical surface 5. FIG. 1 (d) shows the frontier spherical surface 5 and interior spherical surface 6 of the atom 2a, which is extracted from the molecule 1. The frontier spherical surface 5 is a portion exposed to the outside, so that it can be supposed that the frontier spherical surface 5 be a region mainly concerning in a chemical reaction.

Each of the component spaces corresponds to a space surrounded by a surface, which cuts the interior spherical surface 6, and the frontier spherical surface 5.

Then, as shown in FIG, 1 (e), probe points 7 are set on the atomic spherical surface 4 at regular intervals. Each of the probe points 7 is a point for diagnosing the characteristics of the molecule 1 at that position.

In the FRAU, in order to numerically characterize the electronic and steric factors of the molecule 1, three kinds of features are estimated. The three kinds of features include a space occupied rate (FF field), an electrostatic feature (FF electro) ands steric feature (FF steric). These features are

called FRAU features (FF). The FRAU characteristics (FF) are operated for each of the atoms 2a, 2b, 2c, ··· of the molecule 1.

The space occupied rate (FF field) is given as the number of the probe points 7 existing on the frontier spherical surface 5 of each of the atoms 2a, 2b, 2c, ··· . The fact that the space occupied rate (FF field) is large shows that the portion occupied by the characteristic of the corresP0ndin$_9$ atom in the whole reaction characteristic of the molecule 1 is large.

The electrostatic energies between a unit charge set at each of the probe points 7 and charges of all of the atoms 2a, 2b, 2c, ··· of the molecule 1 are derived for each of the probe points 7 on the frontier spherical surface 5 of each of the atoms, and summed up for the probe points 7 on the frontier spherical surface 5 of the corresponding atom to give the electrostatic feature (FFelectro), which is calculated by equation (1).

$$FFelectro = \{ \sum_{i=1}^{FFfield} \sum_{j=1}^{natom} 331.8417 \times charge(j) / r_{ij} \} / FFfield \qquad \text{(kcal/mol) (1)}$$

In the equation (1), natom denotes the number of atoms of the molecule 1, charge (j) denoting the charge of each of the atoms, and FF field denoting the space occupied rate. The fact that the electrostatic factor (FF electro) is large shows that a molecule, which has a positive charge and which is to be reacted

with the molecule 1, is difficult to approach to (or 'attack to') the molecule 1.

The van der Waal's energies between probe atoms having a predetermined steric characteristic set at the probe points 7 and all of the atoms of the molecule are derived for each of the probe points 7 on the frontier spherical surface 5 of each of the atoms, and the steric factor (*FF* steric) is given as the sum of the van der Waals energies on the frontier spherical surface 4 of the corresponding atom. The steric feature (FF steric) is estimated using a mathematical technique for calculating a van der Waals energy in a (well known) molecular force field MM3, and the steric feature (FF steric) is calculated by equation (2)

$$\text{FFsteric} = [\sum_{i=1}^{FFfield}\sum_{j=1}^{natom}\sqrt{\varepsilon_i \times \varepsilon_j}\{1.84\times10^5 \exp(-12.0/\frac{r_i + r_j}{r_{ij}}) - 2.25\times(\frac{r_i + r_j}{r_{ij}})^6\}]/FFfield \quad (\text{kcal/mol}) \qquad (2)$$

For example, sp^3 carbon, sp^2 carbon or sp carbon is preferably used as the probe atom. In the equation (2), sp^3 carbon is used as the probe atom. In the equation (2), Σ denotes a parameter of MM3 indicative of the hardness of an atom, r_i (or r_j) denoting a van der Waals radius defined in the MM3, r_{ij} denoting a distance between a number i probe point and a number j atom on the frontier spherical surface 5 of the corresponding atom. The fact that the steric feature (FFsteric) is large shows

that a molecule to be reacted with the molecule 1 is difficult to approach to (or 'attack to') the molecule 1 since the steric hinderance is large.

Furthermore, in the above description, while the number of probe points 7 existing on the frontier spherical surface 5 of each of the atoms 2a, 2b, 2c, ··· has been adopted as the space occupied rate (FF field), the area of the frontier spherical surface 5 of each of the atoms 2a, 2b, 2c, ··· may be adopted as the space occupied rate (FF field). The adoption of the area of the frontier spherical surface 5 as the space occupied rate (FF field) is useful for the case where the area of the frontier spherical surface 5 is analytically derived.

In the above description, it has been assumed that the molecule surrounding surface 20 be first set so as to be reflected in the spatial dimension of the molecule, and the outermost contour enveloping surface formed by the plurality of atomic spherical surfaces 4 has been adopted as the molecule surrounding surface. However, it may be considered that the atomic spherical surface 4 is derived for each of the plurality of atoms 2a, 2b, 2c, ··· of the molecule 1 using the center of each of the atoms as the center of the spherical surface without the premise that the molecule surrounding surface is first set, so that the molecule surrounding surface is obtained as the

outermost contour *enveloping* surface formed by the plurality of atomic spherical surfaces 4.

In the above description, while the plurality of atomic spherical surfaces 4 have been derived to divide the molecule surrounding space 21intothepluralityofcomponentspaces23, the procedure for spatially dividing the molecule surrounding space 21 into the plurality of component spaces should not be limited thereto.

For example, the molecule surrounding surface 20 may be Voronoi-divided into a plurality of component spaces. In this case, Voronoi-regions obtained by the Voronoi division are used as component spaces 22. For that purpose, a molecule surrounding surface 20 is first set by the frontier molecular orbital of a molecule. Then, in accordance with a technique of Voronoi diagram(e.g., *see ACMC* onputting Surveys, vol.23, no.3 (1991), pp.345-405 (translated into Japanese by Kokichi Sugiharm, Voronoi Diagram-Introduction to One Basic Geometrical Data Structure, bit 1993, Separate Volume of the September Number, Computer Science, Kyoritu Shuppan, Tokyo, 1993, pp.131-185)), the centers of the atoms 2a, 2b, 2c, ··· of the molecule 1 are used as mother points to Voronoi-divide the molecule surrounding space 21 surrounded by the molecule surrounding surface 20 to obtain a Voronoi region for each atom. The contour surface of the obtained Voronoi region comprises a frontier surrounding surface on the molecule

surrounding surface 20, and a boundary surface to the adjacent Voronoi region.

When the Voronoi region is adopted as the component space 22, the Voronoi region is preferably corrected by weighting on the basis of the ratio of the van der Waals radius of each of atoms and Voronoi-dividing in order to reflect the difference in size of the atoms 2a, 2b, 2c, ··· of the molecule 1.

When the Voronoi region is adopted as the component space 22, the quantity for the volume of the Voronoi region is preferably adopted as the space occupied rate (FF field).

If the Voronoi region is adopted as the component space 22 as described above, the following advantages can be obtained. That is, it is possible to select a molecule surrounding space suitable for the object of applying a molecular reaction characteristic predicting method according to the present invention. For example, it is also possible to set a component space for each functional group while reflecting the characteristic of the functional group."

(2) With respect to the Examiner's questions about the Voroni decision, it is important to note that three kinds of features are estimated in the FRAU. The three kinds of features are a space occupied rate (FF field), an electrostatic feature (FF electro) and a steric feature (FF static).

The space occupied rate (FF field) can be estimated for each atom composing the molecule 1 and are given as (for example) the number of the probe points 7 existing on the frontier spherical surface 5 of each of the atoms 2a, 2b, 2c, ····.

Here, the probe points are set on the frontier spherical surface 4 at regular interval of each of the atoms 2a, 2b, 2c, ··. The fact that the space occupied rate (FF field) of the atom is large shows that the atom occupies spacially the large part of the space of the molecule 1.

Applicants have forwarded the requested paper of a Voronoi division, however, it has not arrived due to the current mail situation in Washington, D.C. and will be submitted when received. It must be noted that the Voronoi division is not essential for the present invention, because the Voronoi division is only one embodiment of the procedure for spatially dividing the molecule surrounding space 21 into the plurality of component spaces. For the Examiner's reference Fig.31 in page 380 of the document shows similar procedure for dividing a space.

(3) The fact that the electrostatic factor (FFelectro) of the molecule is large shows that an assumed molecule to be reacted with the molecule 1 and having a positive charge is difficult to approach to (or 'attack to') the molecule 1.

(4) As to "deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said component spaces, as a steric factor of said corresponding one of said component spaces" of claim 1, this corresponds to the formula (2), and the formula (2) is one case where sp^3 carbon is used as the probe atom. The procedure of obtaining the steric feature (FF steric) is described in page 12, line 31 to page 13, line 19.

Trying to estimate the steric feature (FF steric) for the atom 2a, the following procedures are taken: a probe atom such as sp^3 carbon is selected and the probe atom is set on one probe point(i) on the frontier spherical surface 4 of the atom 2a, and the van der Waals energies between the probe atom on the probe point (i) and each of all the atoms 2a, 2b, 2c, ··· are estimated. Next, the probe atom is set on one probe point (k) other than (i) on the frontier spherical surface 4 of the atom 2a, and the van der Waals energies between the probe atom on the probe point (k) and each of all the atoms 2a, 2b, 2c, ··· are estimated. Finally, the van der Waals energies are summed up over the probe points on the frontier spherical surface 4 of the atom 2a, and the steric feature (FF steric) for the atom 2a is obtained.

Similarly, in the case of estimating of the electrostatic factor (FF electro) for atom 2a in the formula (1), the following procedures are taken: a Unit charge is set on one probe point (i)

on the frontier spherical surface 4 of the atom 2a, and the electrostatic energies between the probe atom on the probe point (i) and the partial charge (charge (j)) of each of all the atoms 2a, 2b, 2c, ···. are estimated.

Next, a unit charge is set on one probe point(k) other than (i) on the frontier spherical surface 4 of the atom 2a, and the electrostatic energies between the probe atom on the probe point (k) and the partial charge (charge (j)) of each of all the atoms 2a, 2b, 2c, ··· are estimated. Finally, the electrostatic energies are summed up over the probe points on the frontier spherical surface 4 of the atom2a, and the electrostatic factor (FF electro) for atom 2a for the atom 2a is obtained.

Claim Rejections - 35 USC § 103

The Examiner rejected claims 1, 9-12, 14-16 and 18-20 under 35 U.S.C. § 103(a) as being unpatentable over Jain et al. (J. Med. Chem, 1994). Additionally, the Examiner rejected claims 1, 4, 5, 7-16 and 18-20 under 35 U.S.C. § 103(a) as being unpatentable over Jain et al. (J. Med. Chem, 1994); and further in view of Lavender et al. (IEEE Comp. Graphics & App., 1992) and Chen et al. (Bio. org & Med. Chem. Letters, 1998).

It is respectfully submitted that the present claimed invention is patentable over the art of record for the following

reasons. Accordingly, reconsideration of the Examiner's rejection is requested.

The characteristic features of the present invention can be understood by comparing it with the prior art described in page 1, line 27 to page 8, line 17. Here, Jain et al cited in the Office Action can be said to belong to "CoMFA" in the means that a common skeleton is necessary as a common portion in the molecules to be compared and the common skeleton is the dominant part of the molecules.

"In the field of development of medicines, the cooperative molecular field analysis (CoMFA) method is conventionally known as a method for predicting the activity characteristics of ligand molecules (see, e.g., R.D. III Cramer, et al., J. Am. Chem. So., 1988, 100, 5959).

In the CoMFA method, a CoMFA field is produced to five the three-dimensional expression of a chemical structure of ligand molecule. The CoMFA field is derived by forming, e.g., a rectangular parallelepiped-shaped region surrounding a molecule, the activity characteristic of which is to be predicted considering lattice points, which are distributed in the surrounding region in the form of a lattice, as probe points, and putting probe atoms at the respective probe points to calculate energy of the interaction between the probe atoms and the components of the molecule, such as substituents.

In the CoMFA method, it is assumed that a portion occupying a major part of a molecule, the reaction characteristic of which is to be predicted, is a common skeleton serving as a common portion, and the substituted portions of molecules having a common skeleton are substituted by various substituents. On the basis of the correlation characteristics of the obtained CoMFA, the presence of similarity between the activity characteristics of the molecules having the common skeleton is determined.

However, in the CoMFA method, it is assumed that the molecules have the common skeleton, and when the prediction of the activity characteristic of a certain molecule is intended, the presence of similarity between activity characteristics is determined only between the certain molecule and another molecule having a common skeleton with the certain molecule.

Thus, it is not possible to determine the presence of similarity between reaction characteristics of molecules, which have quite different sizes and which do not have any common skeleton.

In addition, in the CoMFA method, a molecule, the reaction characteristic of which is to be predicted, is not decomposed into minute sites to derive characteristic values for each site, and one CoMFA field is obtained as the whole molecule. Therefore, it is not known how each of the sites of the molecule contributes to the reaction, so that it is not possible to

accurately predict and consider the reaction characteristic of the molecule.

Moreover, in the CoMFA method, the rectangular parallelepiped surrounding the overlapped ligand molecules is different in accordance with the size of a target ligand molecule group, so that there is a limit that the obtained characteristic value depends on the target ligand molecule group.

In addition, the CoMFA method is applied to the prediction of activity and the design of a medicine in the development of the medicine, so that the CoMFA method can not be applied to the prediction of reactivity and the design of synthesis in the field of synthetic chemistry. There is no reaction characteristic predicting method serving as a guide to the prediction of reactivity and the design of synthesis in the field of synthetic chemistry and as a guide to the prediction of activity and the design of a medicine in the development of the medicine.

It is therefore an object of the present invention to eliminate the aforementioned problems and to provide a molecular reaction characteristic predicting method, which can be applied to a wide field of chemistry including the field of synthetic chemistry as well as the field of development of medicines and which can accurately predict the presence of similarity between reaction characteristics of various molecules without limitations

on common skeleton, and a reaction characteristic predicting map and computer-readable storage medium.

As shown above, in the case of Jain et al. (CoMFA), it is needed that the skeleton is common between the two molecules to be compared. As shown in Fig. 1 in Jain et al, the two molecules to be compared are positioned so that the two skeletons are superimposed with each other in the rectangular coordinate space where lattice points are distributed as probe points.

The present invention is very different from the case of Jain et al (CoMFA).

In the case of the present invention, for example, there is no procedure to position for superimposing two molecules to be compared and there is no need to set lattice points distributed as probe points in the rectangular coordinate space.

In the case of the present invention, it is possible to compare whether there is similarity between reaction characteristics of molecules having quite different sizes and having no any common skeleton.

Some of the important features in claim 1 exist in "component space". Each "component space" includes on atom composing the molecule.

"A frontier surrounding surface" is defined as a component surrounding surfaces of each of said component spaces appearing outside on said molecule surrounding surface.

Each of "component spaces" having "a frontier surrounding surface" can show a guideline for estimating a reaction characteristics of the molecule. Then, it becomes possible to refer each of the component spaces individually as a guideline for estimating a reaction characteristics of the molecule.

The Examiner cited "the use of neural network" and "the Voronoi diagram" and mentioned to these. However, the Examiner seems to cite these terms only based on the fact she can find out these in the citation having the same technical field as to the present invention.

For example, the neural network is used for grouping the characteristic data in the present invention, but the neural network is used for positioning two molecules to be interposed in the citation, and the neural network is used in much different way between the present invention and the citation.

As shown in claim 8, " the Voronoi diagram" is introduced as on embodiment of said predetermined space dividing procedure 2 in claim 1.

The Examiner's assertion that one of ordinary skill would be motivated to form Applicants' claimed invention is respectfully incorrect. As the Examiner well knows, obviousness cannot be established by combining pieces of prior art absent some teaching, suggestion, or incentive supporting the combination.

Accordingly, in view of the foregoing amendments and remarks, the Examiner is respectfully requested to reconsider and withdraw the rejection of the claims to allow these claims and to find this application to be in allowable condition.

If the Examiner believes that a further conference would be of value in expediting the prosecution of this application, the Examiner is invited to telephone the undersigned to arrange for such a conference.

Attached hereto is a marked-up version of the changes made to the claims by the current amendment. The attached page is captioned "**Version with markings to show changes made.**"

Respectfully submitted,

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Atty. Docket: P63431US0

Version with markings to show changes made.

In the Specification:

Please replace the formula on page 13 lines 5-8 with the following formula:

$$FF_{\text{steric}} = [\sum_{i=1}^{FFfield} \sum_{j=1}^{natom} \sqrt{\varepsilon_i \times \varepsilon_j} \{1.84 \times 10^5 \exp(-12.0 / \frac{r_i + r_j}{r_{ij}})$$

$$- 2.25 \times (\frac{r_i + r_j}{r_{ij}})^6\}] / FFfield \quad \text{(kcal/mol)} \qquad (2)$$

In the Abstract:

Please insert the Abstract of Disclosure, attached as a separate sheet, at the end of the specification.

In the Claims:

Please amend claims 1 and 18-20 as follows:

1. (Amended) A molecular reaction characteristic predicting method for predicting a reaction characteristic of a molecule, said method comprising the steps of:

setting a molecule surrounding surface surrounding the molecule so as to be reflected in a spatial dimension of [a] the molecule, and assuming that a space surrounded by said molecule surrounding surface is a molecule surrounding space;

dividing said molecule surrounding space into a plurality of component spaces, by which a reaction characteristic of said

molecule is characterized, in accordance with a predetermined space dividing procedure, and assuming that contour surfaces surrounding said component spaces are component surrounding surfaces, said molecule surrounding space being divided so as that each component space of the plurality of component spaces includes therein each one atom composing the molecule;

assuming that a portion of each of said component surrounding surfaces appearing outside on said molecule surrounding surface is a frontier surrounding surface of each of said component spaces;

providing probe points on said frontier surrounding surface of each of said component spaces at regular intervals;

deriving a rate of said molecule surrounding space occupied by each of said component spaces, as a space occupied rate of each of said component spaces;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and

deriving the sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said component spaces, as an electrostatic factor of said corresponding one of said component spaces;

deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said component spaces, as a steric factor of said corresponding one of said component spaces; and

assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said component spaces, and predicting a reaction characteristic of said molecule on the basis of said reaction characteristic values of each of said component spaces.

18. (Amended) A molecular reaction characteristic predicting method comprising the steps of:

describing atomic spherical surfaces, each of which surrounds a corresponding one of atoms of a molecule;

assuming that a portion of each of said atomic spherical surfaces intersecting the atomic spherical surfaces of other atoms of said molecule is an interior spherical surface;

assuming that a portion of each of said atomic spherical surfaces other than said interior spherical surface is a frontier

spherical surface, the frontier spherical surface being appeared outside;

providing probe points on each of said atomic spherical surfaces at regular intervals;

deriving a rate of occupied space as a space occupied rate of a corresponding one of said atoms, for each of said atoms;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of said atoms of said molecule, for each of said probe points on said frontier spherical surface of each of said atoms;

deriving the sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said atoms, as an electrostatic factor of said corresponding one of said atoms;

deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said atoms;

deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said atoms, as a steric factor of said corresponding one of said atoms;

assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said atoms; and

predicting a reaction characteristic of said molecule on the basis of said reaction characteristic values of each of said atoms.

19. (Amended) A reaction characteristic predicting map for predicting a reaction characteristic of a molecule, wherein referring to a molecular reaction characteristic predicting method for predicting a reaction characteristic of a molecule, said method comprising the steps of:

setting a molecule surrounding surface so as to be reflected in a spatial dimension of a molecule, and assuming that a space surrounded by said molecule surrounding surface is a molecule surrounding space;

dividing said molecule surrounding space into a plurality of component spaces, by which a reaction characteristic of said molecule is characterized, in accordance with a predetermined space dividing procedure, and assuming that contour surfaces surrounding said component spaces are component surrounding surfaces, said molecule surrounding space being divided so as that each component space of the plurality of component spaces includes therein each one atom composing the molecule;

assuming that a portion of each of said component surrounding surfaces appearing outside on said molecule surrounding surface is a frontier surrounding surface of each of said component spaces;

providing probe points on said frontier surrounding surface of each of said component spaces at regular intervals;

deriving a rate of said molecule surrounding space occupied by each of said component spaces, as a space occupied rate of each of said component spaces;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said component spaces, as an electrostatic factor of said corresponding one of said component spaces;

deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said van der Waals energies on said frontier surrounding surface

of said corresponding one of said component spaces, as a steric factor of said corresponding one of said component spaces; and

assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said component spaces, and predicting a reaction characteristic of said molecule on the basis of said reaction characteristic values of each of said component spaces;

said space occupied rate, said electrostatic factor and said steric factor are derived for each of said component spaces forming said molecular surrounding space of each of a plurality of molecules, the reaction characteristics of which are to be predicted,

a plurality of sets of input data are generated so as to correspond to said plurality of component spaces of each of said plurality of molecules, each set of said plurality of sets of input data being formed by said space occupied rate, said electrostatic factor and said steric factor,

said plurality of sets of generated input data are processed in accordance with a technique of a self-organizing neural network, and

the processed result is displayed so as to indicate reaction characteristics of said plurality of molecules.

20. (Amended) A computer-readable storage medium having stored a program for predicting a reaction characteristic of a molecule, said program carrying out a process comprising the steps of:

setting a molecule surrounding surface surrounding the molecule so as to be reflected in a spatial dimension of a molecule, and assuming that a space surrounded by said molecule surrounding surface is a molecule surrounding space;

dividing said molecule surrounding space into a plurality of component spaces, by which a reaction characteristic of said molecule is characterized, in accordance with a predetermined space dividing procedure, and assuming that contour surfaces surrounding said component spaces are component surrounding surfaces, said molecule surrounding space being divided so as that each component space of the plurality of component spaces includes therein each one atom composing the molecule;

assuming that a portion of each of said component surrounding surfaces appearing outside on said molecule surrounding surface is a frontier surrounding surface of each of said component spaces;

providing probe points on said frontier surrounding surface of each of said component spaces at regular intervals;

deriving a rate of said molecule surrounding space occupied by each of said component spaces, as a space occupied rate of each of said component spaces;

deriving electrostatic energies between a unit charge set at each of said probe points and charges of all of atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said electrostatic energies on said frontier surrounding surface of a corresponding one of said component spaces, as an electrostatic factor of said corresponding one of said component spaces;

deriving van der Waals energies between a probe atom, which is set at each of said probe points and which has a predetermined steric characteristic, and all of said atoms of said molecule, for each of said probe points on said frontier surrounding surface of each of said component spaces, and deriving the sum of said van der Waals energies on said frontier surrounding surface of said corresponding one of said component spaces as a steric factor of said corresponding one of said component spaces; and

assuming that said space occupied rate, said electrostatic factor and said steric factor are reaction characteristic values of said corresponding one of said component spaces, and predicting a reaction characteristic of said molecule on the basis of said reaction characteristic values of each of said component spaces.